

# **Quick-Reference Card**

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### Help and information.

helppls - Context related help on the PLS Toolbox.

demos - Demo list for the PLS Toolbox.

evridebug - Checks the PLS Toolbox installation for problems.

evriinstall - Install Eigenvector Research Product.

evriuninstall - Uninstall an Eigenvector Research toolbox.

evriupdate - Check Eigenvector.com for available PLS Toolbox updates.

plsver - Displays version information.

<functionname> io - Prints short version of the io.

<functionname> help - Accesses the online help.

## Plotting, Analysis Aids, and I/O Functions.

abline - Draws a line on the current axes with a given slope and intercept.

areadr - Reads ascii data and strips header.

autoimport - Automatically imports all standard filetypes.

builddbstr - Builds a database connection string.

dp - Draws a diagonal line on an existing figure.

ellps - Plots an ellipse on an existing figure.

**explode** - Extracts variables from a structure array to the workspace.

getpidata - Uses the current PI connection to construct a DSO. **gselect** - Selects objects in a figure (various selection styles).

hline - Adds horizontal lines to figure at specified locations.

infobox - Display a string in an information box.

loopfilereadr - An example function for reading files in a loop from a directory.

mplot - Automatic creation of subplots and plotting.

mtfreadr - Read AdventaCT Multi-Trace Format (MTF) files.

parsemixed - Parse numerical and text data into a DataSet Object.

pcolormap - Pseudocolor plot with labels and colorbar.

ploteigen - Builds dataset object of eigenvalues/RMSECV information.

plotgui - Interactive data viewer.

plttern - Plots a 2D ternary diagram.

pltternf - Plots a 3D ternary diagram with frequency of occurrence.

querydb - Executes a query on a database defined by connection string.

rwb - Red white and blue color map.

setpath - Modifies and saves current directory to the MATLAB search path.

spcreadr - Reads a Galactic SPC file.

trendtool - Univariate trend analysis tool.

vline - Adds vertical lines to figure at specified locations.

writecsy - Export a DataSet object to a comma-separated values (CSV) file.

xclgetdata - Extracts matrix from an Excel spreadsheet.

xclputdata - Write matrix to an Excel spreadsheet.

xclreadr - Reads an ASCII or .XLS file in as a DataSet Object.

xlsreadr - Reads .XLS files from MS Excel and other spreadsheets.

xyreadr- Reads one or more ASCII XY or XY... files

vscale - Rescales the y-axis limits on each subplot in a figure.

**zline** - Adds vertical lines to 3D figure at specified locations.

# Data Editing, Scaling, and Preprocessing.

auto - Autoscales matrix to mean zero unit variance.

baseline - Subtracts a polynomial baseline offset from spectra.

baselinew - Baseline using windowed polynomial filter.

coadd - Reduce resolution through combination of adjacent variables or samples.

delsamps - Deletes samples (rows) or variables (columns) from data matrices

editds - Editor for DataSet Objects.

glsw - Generalized least-squares weighting/preprocessing.

gscale - Group/block scaling for a single or multiple blocks.

gscaler - Applies group/block scaling to submatrices of a single matrix.

lamsel - Determines indices of wavelength axes in specified ranges. logdecay - Mean centers and variance scales a matrix using the log decay of the variable axis.

**lsq2top** - Fits a polynomial to the top/(bottom) of data.

mdcheck - Missing Data Checker and infiller.

med2top - Fits a constant to top/(bottom) of data.

medon - Median center scales matrix to median zero.

mncn - Scale matrix to mean zero.

mscorr - Multiplicative scatter/signal correction (MSC).

normaliz - Normalize rows of matrix.

oscapp - Applies OSC model to new data.

osccalc - Calculates orthogonal signal correction (OSC).

polyinterp - Polynomial interpolation, smoothing, and differentiation. preprocess - Selection and application of standard preprocessing

structures.

preprouser - User-defined preprocessing methods.

registerspec - Shift spectra based on expected peak locations.

rescale - Scales data back to original scaling.

savgol - Savitzky-Golay smoothing and differentiation.

savgolcv - Cross-validation for Savitzky-Golay smoothing and differentiation.

scale - Scales data using specified means and std. devs.

shuffle - Randomly re-orders matrix and multiple blocks rows.

sny - Standard normal variate scaling.

specedit - GUI for selecting spectral regions on a plot.

super reduce - Eliminates highly correlated variables.

unfoldm - Rearranges (unfolds) an augmented matrix to row vectors.

unfoldmw - Unfolds multiway arrays along specified order.

wlsbaseline - Weighted least squares baseline function.

# Statistics, ANOVA, Experimental design.

anova1w - One-way analysis of variance.

anova2w - Two-way analysis of variance.

corrmap - Correlation map with variable grouping.

distslct - Selects samples on outside of data space.

doptimal - Selects samples based on D-Optimal criteria.

durbin watson - Criterion for measure of continuity.

factdes - Full factorial design of experiments.

ffacdes1 - Fractional factorial design of experiments.

ftest - F test and inverse F test statistic.

percentile - Finds percentile point (similar to MEDIAN).

stdsslct - Selects data subsets (often for use in standardization).

ttesto - Evaluates t-distribution and its inverse.

### **Principal Components Analysis**

chilimit - Chi-squared confidence limits from sum-of-squares residuals.

datahat - Calculates the model estimate and residuals of the data. estimatefactors - Estimate number of significant factors in

multivariate data. imlimit - Confidence limits for Q residuals via Jackson-Mudholkar. mlpca - Maximum likelihood principal components analysis.

pca - Principal components analysis.

pcaengine - Principal Components Analysis computational engine.

pcapro - Projects new data on old principal components model. plotloads - Extract and display loadings information from a model structure.

plotscores - Extract and display score information from a model. residuallimit - Estimates confidence limits for sum squared residuals. ssgtable - Displays variance captured table for model.

subgroupcl - Displays a confidence ellipse for points in a twodimensional plot.

tsalim - Confidence limits for Hotelling's T^2.

tsamtx - Calculates matrix for T^2 contributions for PCA.

varcap - Variance captured for each variable in PCA model.

varimax - Orthogonal rotation of loadings.

# **Curve Resolution and Evolving Factor Analysis**

als - Alternating Least Squares computational engine. comparelcms simengine - Calculational Engine for comparelcms. comparelcms sim interactive - Interactive interface for COMPARELCMS.

coda\_dw\_interactive - Interactive version of CODA DW. coda dw - Calculates values for the Durbin Watson criterion of columns of data set.

evolvfa - Evolving factor analysis (forward and reverse).

ewfa - Evolving window factor analysis.

mcr - Multivariate curve resolution with constraints.

purity - Self-modeling mixture analysis method based on purity of variables or spectra.

purityengine - calculates purity values of columns of data set. wtfa - Window target factor analysis.

### **Cluster Analysis and Classification Functions**

class2logical - Create a PLSDA logical block from class assignments.

cluster - KNN and K-means cluster analysis with dendrograms.

acluster - GUI function for use with CLUSTER. discrimprob - Discriminate probabilities for continuous predicted values.

knn - K-nearest neighbor classifier.

plsda - Partial least squares discriminant analysis.

plsdaroc - Calculate and display ROC curves for PLSDA model.

plsdthres - Bayesian threshold determination for PLS Discriminate

simca - Soft Independent Method of Class Analogy.

### **Multi-way and Image Functions**

alignmat - Alignment of matrices and N-way arrays. corcondia - Evaluates consistency of PARAFAC model. coreanal - Analysis of the core array of a Tucker model. corecalc - Calculate the Tucker3 core given the data array and loadings.

gram - Generalized rank annihilation method. modelviewer - Visualization tool for multi-way models. mpca - Multi-way (unfold) principal components analysis. nassign - Generic subscript assignment indexing for n-way arrays. ncrossval - Cross-validation for multilinear PLS (N-PLS). nindex - Generic subscript indexing for n-way arrays. npls - Multilinear-PLS (N-PLS) for true multi-way regression. **npreprocess** - Preprocessing of multi-way arrays. outerm - Computes outer product of any number of vectors. parafac - Parallel factor analysis for n-way arrays. parafac2 - Parallel factor analysis for unevenly sized n-way arrays. tld - Trilinear decomposition.

### Linear and Non-Linear Regression.

tucker - Analysis for n-way arrays.

cr - Continuum Regression for multivariate v. crcvrnd - Cross-validation for continuum regression.

crossval - Cross-validation for decomposition and linear regression.

fastnnls - Fast non-negative least squares.

figmerit - Analytical figures of merit for multivariate calibration.

frpcr - Full-ratio PCR calibration and prediction.

frocrengine - Engine for full-ratio PCR regression.

leverag - Calculate sample leverages.

lwrpred - Predictions based on locally weighted regression models. lwrxy - Predictions based on lwr models with v-distance weighting. mlr - Multiple Linear Regression for multivariate Y.

mlrengine - Multiple Linear Regression computational engine.

modlpred - Predictions using standard model structures.

modirder - Displays model info for standard model structures.

nippls - NIPALS Partial Least Squares computational engine.

pcr - Principal components regression for multivariate Y.

pcrengine - Principal Component Regression computational engine.

pls - Partial least squares regression for multivariate Y.

plsnipal - NIPALS algorithm for one PLS latent variable.

polypls - PLS regression with polynomial inner-relation.

**regcon** - Converts regression model to y = ax + b form.

ridge - Ridge regression by Hoerl-Kennard-Baldwin.

ridgecy - Ridge regression by cross validation.

rinverse - Calculate pseudo inverse for PLS, PCR and RR models.

rmse - Calculate Root Mean Square Error.

simpls - Partial Least Squares computational engine using SIMPLS algorithm.

varcapy - Calculate percent y-block variance captured by a PLS regression model.

vip - Calculate Variable Importance in Projection from regression model.

#### Multivariate Instrument Standardization.

caltransfer - Create or apply calibration and instrument transfer models.

deresoly - Changes high resolution spectra to low resolution. stdfir - Standardization based on FIR modelling.

stdgen - Piecewise and direct standardization transform generator.

stdize - Applies transform from STDGEN to new spectra.

#### Variable Selection

calibsel - Statistical procedure for variable selection. fullsearch - Exhaustive Search Algorithm for small problems. gaselctr - Genetic algorithm for variable selection with PLS. genalg - Genetic Algorithm for Variable Selection. genaloplot - Plot GA results using selected variable plot, color-coded by RMSECV.

ipls - Interval PLS variable selection.

# MSPC and Finite Impulse Response Models.

autocor - Auto-correlation function for time series data. crosscor - Cross-correlation function for time series data. fir2ss - Transform FIR model into equivalent state space model. plspulsm - Identifies FIR dynamics models for MISO systems. plsrsqcv - Generate PLS models for MSPC with cross-validation. plsrsqn - Generates a matrix of PLS models for MSPC. replace - Replaces variables based on PCA or PLS models. wrtpulse - Create input/output matrices for dynamic model identification.

#### **Model Utilities**

browse - PLS Toolbox Toolbar and Workspace browser.

choosencomp - GUI to select number of components from SSQ table

compressmodel - Remove references to unused variables from a model.

copydsfields - Copies informational fields between datasets and/or models.

matchyars - Align variables of a dataset to allow prediction with a model.

modelselector - Create or apply a model selector model.

modelstruct - Constructs an empty model structure.

reviewmodel - Examines a standard model structure for typical problems.

updatemod - Update model structure to be compatible with the current version.

# **Programming Utilities**

besttime - Returns a string describing the time interval provided (in seconds).

comparevars - Compares two variables of any type.

encode - Translates a variable into matlab-executable code. erdiapis - Error dialog.

evrirelease - Returns Eigenvector product release number.

exportfigure - Automatically export figures to an external program.

figbrowser - Browser with icons of all Matlab figures.

findindx - Finds the index of the array element closest to value r.

**getdatasource** - Extract summary dataset info.

getmiversion - Returns current Matlab version as an integer.

getplspref - Get overriding options (preferences) for PLS Toolbox functions.

Iddiapls - Dialog to load variable from workspace or MAT file.

moveobj - Interactively reposition graphics objects.

helppls - Context related help on the PLS Toolbox.

reversebytes - Flips order of bytes in a word.

setplspref - Set overriding options (preferences) for PLS Toolbox functions.

string x - Add backslash before troublesome TeX characters. sydlapls - Dialog to save variable to workspace or MAT file.

### PLS Toolbox Demonstrations.

datasetdemo - Demonstrates use of the dataset object. demos - Demo list for the PLS Toolbox. linmodeldemo - Demo of the CROSSVAL, MODLRDER, PCR, PLS, PREPROCESS and functions.

<functionname> demo - Runs a short demo for each function.

projdemo - Demo of the MLR, PCR, and PLS regression vectors.

statdemo - Elementary stats, t test, F test and AVOVA.

stddemo - Demo of the STDSSLCT. STDGEN, and OSCCALC functions

# PLS Toolbox Test Data Sets.

**alcohol** - Biological fluid analysis of alcoholics for discriminant analysis.

aminoacids- Fluorescence EEM of 5 samples for PARAFAC. arch- Archeological artifact data set for PCA amd SIMCA examples.

bread - Sensory evaluation of breads.

dorrit- EEM of 27 samples with 4 flourophores for PARAFAC.

etchdata - Data from semiconductor metal etch.

fia - Flow Injection Analysis of hydroxy-benzaldehydes.

halddata - Hald cement curing data.

nir data - NIR spectra of pseudo gasoline samples for STDDEMO.

nmr data - NMR data for GRAM demo.

oesdata - Optical emission spectra from metal etch.

paint - Non-linear paint formulation data.

pcadata - Slurry Fed Ceramic Melter data.

plsdata - SFCM data for PCR and PLS demos.

pisiogo - Generates PLS Toolbox CR surface logo.

proidat - Projection demo data for PROJDEMO.

pulsdata- Time series data for PLSPULSM demo.

replacedata - SFCM data for REPLACEDEMO.

sawdata - Surface acoustic wave sensor data for organic vapors.

smbread - Images of bread at 5 wavelengths.

statdata- Data sets for ANOVA and statistics STATDEMO.

sugar - Fluorescence EEM N-way data set.

wine- Wine data set for PCA example.

areadrdemtext.txt - Text file used by AREADRDEMO.

xclreadrdata.txt- Text file used by XCLREADRDEMO.

Redbeerdata.xls - Example spreadsheet for "Intro to MATLAB".

#### Frequently Asked Questions:

http://software.eigenvector.com/fag/

#### Request Help at:

helpdesk@eigenvector.com

#### Send the output of the commands:

evridebua ver path

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